Piperazine

110-85-0 | DTXSID1021164

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.20

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 5.92e-01

Nearest Neighbors from the Training Set

Image not found

Piperazine
Measured: -1.50
Predicted: -1.20

Image not found

Morpholine
Measured: -0.860
Predicted: -0.646

Image not found

N-Nitrosopiperazine
Measured: 0.18
Predicted: -0.0453

Image not found

N-Nitrosomorpholine
Measured: -0.440
Predicted: -0.463

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N,N'-Dimethylethane-1,2-diamine
Measured: -0.620
Predicted: -0.629